Screening Peptida Siklis komersial sebagai inhibitor Protein Envelope Denv melalui Molecular Docking dan Molecular Dynamics = Screening of commercial cyclic peptides as inhibitor envelope Protein Denv through Molecular Docking and Molecular Dynamics

Kinanty, author

Abstrak

Virus dengue (DENV) telah menyebar luas di berbagai penjuru dunia, terutama pada daerah beriklim tropis. Pengobatan yang efektif terhadap infeksi DENV belum tersedia walaupun telah dikembangkan beberapa kandidat vaksin. Pengobatan yang dilakukan saat ini hanya untuk mengurangi gejala sakit dan mengurangi risiko kematian. Oleh karena itu, dibutuhkan suatu pengobatan yang bersifat antiviral. Protein envelope merupakan salah satu protein struktural DENV yang diketahui dapat menjadi target inhibitor antiviral dan berperan khusus dalam proses fusi.

Penelitian ini bertujuan untuk screening peptida siklis komersial yang digunakan sebagai inhibitor protein envelope DENV melalui molecular docking dan molecular dynamics pada temperatur 310K dan 312K. Screening 301 peptida siklis komersial melalui molecular docking menghasilkan 10 ligan terbaik dan berdasarkan interaksi ikatan hidrogen dan kontak residu pada cavity protein envelope didapatkan tiga ligan terbaik yang dapat memasuki cavity protein envelope secara keseluruhan. Ketiga ligan tersebut diuji melalui ADME-Tox dan didapatkan ligan terbaik, yaitu BNP (7-32), porcine. Hasil simulasi molecular dynamics pada temperatur 310K dan 312K menunjukan bahwa ligan dapat mempertahankan interaksi dengan cavity target, sehingga ligan BNP (7-32), porcine dapat dijadikan kandidat antiviral untuk DENV.

.....Dengue virus (DENV) has spread throughout the world, especially in tropical climates. Effective treatment of DENV infection is not yet available although several candidate vaccines have been developed. Treatment at this time is only to reduce symptoms and reduce the risk of death. Therefore, antiviral treatment is very needed. Envelope Protein is one of the structural proteins of DENV which is known could be a target of antiviral inhibitors and plays a special role in the fusion process.

This research aims to screen the commercial cyclic peptides which are used as inhibitors of envelope protein DENV through molecular docking and molecular dynamics at 310K and 312K. Screening of commercial cyclic peptides through molecular docking ligands obtained best 10 ligands then examined the interaction between hydrogen bonding and residue contacts of the cavity envelope protein and obtained best three ligands which could enter the cavity of envelope protein overall. The three ligands were predicted through the ADME-Tox and obtained the best ligands, namely BNP (7-32), porcine. The results of molecular dynamics simulations at 310K and 312K revealed that ligand can maintain interaction with the cavity of the target.